Correlation of CN/C_2 Ratios to Ultrananocrystalline Diamond (UNCD) Film Properties in Microwave Plasmas

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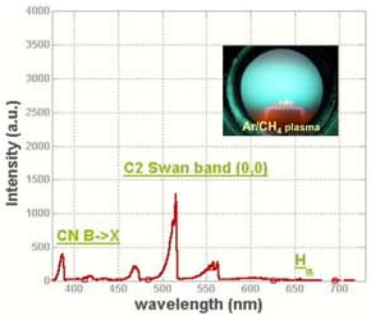
Introduction

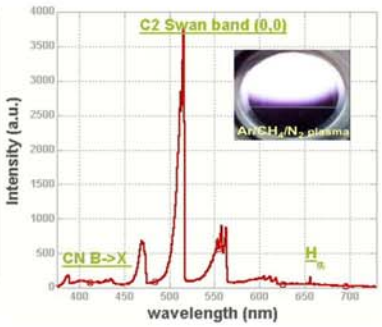
- UNCD thin films consist of 2-5 nm grains of pure sp^3-bonded carbon and 0.5 nm wide grain boundaries (GB).
- Such films have interesting properties closely connected to their unique nanoscale morphology and electronic structure.
- The addition of nitrogen to the CH_4/Ar synthesis gas, has a profound impact on UNCD film electrical conductivity leading to the **highest known ambient temperature *n*-type conductivity of any diamond thin film.**

Major accomplishments

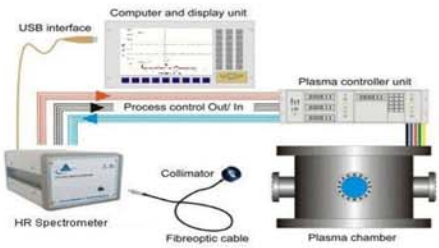
- **Optical Emission Spectroscopy (OES) study of CN/C_2 ratios as a function of nitrogen content and chamber pressure** has been conducted on the plasma phase of a conventional MW CH_4-Ar-rich gas mixture used for UNCD film deposition.



OES Ar-CH_4 plasma
100 Torr, 800 W, 800 °C



OES Ar-CH_4-N_2 plasma
100 Torr, 800 W, 800 °C



OES experimental setup

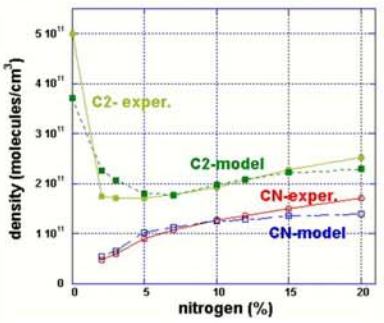
- At measured gas temperature of 1600 K for these plasmas, a substantial fraction of the CH_4 in the feed gas is thermally converted into C_2H_2 that in presence of nitrogen will form HCN.
- We proposed a **thermodynamic equilibrium reaction** to explain the decreases in C_2 and increases in CN concentrations observed in the OES analysis:

(1) $C_2H_2+N_2 \rightarrow 2HCN$ $K_{eq}=0.15$

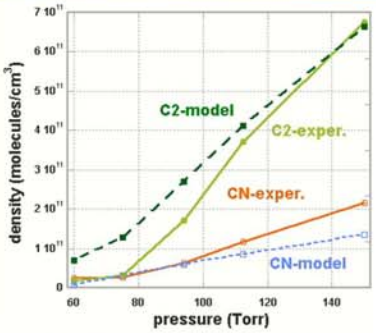
(2) $2HCN \rightarrow C_2N_2+H_2$ $K_{eq}=6.47e\text{-}3$

and **a plasma chemistry model**:

O.A. Williams et al., Applied Physics Letters 85, 1680 (2004).



Simulated (- - - curve) and experimental (—— line) plots as a function of the N_2 addition to the plasma phase.

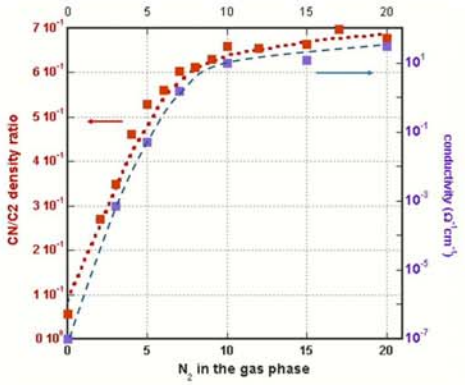


Simulated (- - - curve) and experimental (—— line) plots as a function of total chamber pressure.

Model works !!!!

- C_2 comes both from the fragmentation of C_2H_2 and C_2N_2 and that CN comes from the fragmentation of both HCN and C_2N_2, as predicted from the model.

Correlation CN/C_2 ratio with film properties



CN/C_2 density ratio and conductivity as a function of N_2 in the plasma.

log (*K*·Conductivity) ≈ CN/C_2

Significance

- For the first time a very strong correlation has been observed between the OES results on the plasma used for UNCD deposition and the film electrical properties itself.

Future directions

- Further investigations in order to explain the correlation pointed out between the plasma phase and the electrical conductivity.
- Development of a coherent theory able to explain the electrical conductivity observed in n-type UNCD films as nitrogen is added to the plasma.
- Future implements of n-type UNCD films in electronic applications.

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